

LUIA (Library User Interface for Sensitivity Analysis): a generic software component for sensitivity analysis of bio-physical models

Donatelli, M.^{1,3}, **R. Confalonieri**², **I. Cerrani**³, **D. Fanchini**³, **M. Acutis**², **S. Tarantola**⁴, **B. Baruth**³

¹ Agriculture Research Council; Center of Research for Industrial Crops, currently seconded to 3

² University of Milan, Department of Crop Science

³ European Commission, Joint Research Centre, Institute for the Protection and Security of the Citizen, Agriculture Unit, AGRI4CAST Action

⁴ European Commission, Joint Research Centre, Institute for the Protection and Security of the Citizen, Technological and Economic Risk Management Unit, STAT-IND Action

Email: marcello.donatelli@jrc.it

Abstract: Sensitivity analysis is crucial for a better understanding of model behavior, both for developers and users. Developers can be supported in avoiding over parameterizations and in focusing their attention only on the processes with a significant impact on the output(s) of interest. Model users can benefit from sensitivity analysis by identifying the most relevant parameters in a specific either biophysical or physical context and, therefore, in optimizing the available resources for determining their values, by direct measurements or calibration. When biophysical, deterministic models are run with stochastic data like weather of climate ensembles, and when other inputs, such as management actions, of a model vary substantially, the results of a sensitivity analysis may provide information about different, site specific strategies for operational use. The availability of a generic software component integrated into the modeling and simulation software environment would hence allow the estimation of differences in the behavior of models in different contexts.

It is possible to classify the methods for sensitivity analysis developed in the last decades in three groups: the one-factor-at-a-time method, the methods based on regression and the variance-based Monte-Carlo methods. The first group is represented as an example by Morris' method, which calculates two metrics: the average (μ) and the standard deviation (σ) of the population of the incremental ratios according to an opportune generation of a sample of the possible combination of parameters. The most famous methods belonging to the second group are the Latin Hypercube, the Random and the Quasi-random Lp-Tau. They differ in the method used for generating the sample, while are all based on a linear regression between the differences in the outputs of the model and those in the values of parameters to calculate sensitivity indices. The third group is based on the decomposition of the total variance in terms of increasing dimensionality and it is able to quantify the effect of the interactions among parameters. The methods based on this principle are Fourier Amplitude Sensitivity Test (FAST), Extended FAST, and Sobol's method. The last group, and in particular Sobol's method, is considered the most powerful and precise in identifying the sensitivity of the model output, in response to changes in model parameters. Their drawback is the computational cost since they involve the estimation of k-dimensional integrals. On the other hand, the first group methods are the one requiring the smallest sample for ranking the parameters according to their relevance and it is considered particularly suitable for preliminary screenings of models with several parameters.

This paper describes the LUIA (Library User Interface for Sensitivity Analysis) component, based on the SimLab (<http://simlab.jrc.ec.europa.eu/>) C++ DLL. LUIA has been developed in C# under the .NET platform, with the goal to facilitate the integration of sensitivity analysis capabilities into bio-physical model frameworks. To provide illustrative case studies, a spatially distributed sensitivity analysis of two different biophysical models was carried out using the MARS database (<http://mars.jrc.ec.europa.eu/>), covering the pedo-climatic conditions of Europe. The two models used were the WARM model for rice simulations and the generic crop simulator CropSyst with a parameterization for wheat. Results are presented and discussed according to the spatial variability of parameter relevance.

Keywords: *SimLab, WARM, rice, CropSyst, wheat, Morris*

1. INTRODUCTION

Mathematical models are the primary way to estimate the effect of multiple factors on biophysical systems. They quantify system performances, and their outputs are based on mathematical structure, biophysical input data, and a set of parameters which values describe the system being simulated. Biophysical models are always simplifications of the real systems under study. Even if assumptions and inputs reflect – or are at least representative of – conditions believed to be true, they are always uncertain to some degree, depending on the variability of input data and parameters.

Sensitivity analysis (SA) is a fundamental tool in the building, use and understanding of mathematical models of all forms (Tarantola and Saltelli, 2003). SA provides information about the behaviour of the simulated system ranging from the identification of relevant model factors (parameters or inputs) to model reduction or simplification, to better understanding of the model structure for given components of a system, and to model quality assurance, hence to model building/development in general. Simple SA procedures can be used to illustrate either graphically or numerically the consequences of alternative assumptions about input factors. While in uncertainty analysis the goal is evaluating probabilities of occurrence of model outputs as a response to variability in inputs, in SA the focus is on the analysis of model structure and behaviour. SA thus measures the change in the model output in a localized region of the input factors' space (as generated from the distributional range of values). The exact character of a SA depends upon the particular context and the questions of concern. Sensitivity studies can provide a general assessment of the variability of model output (model precision) when used to assess system capability for alternative combinations of factors, as well as detailed information addressing the relative significance of errors in various factors.

As a consequence, sensitivity results should be of interest to the general public, local and national management agencies, natural resources planners and managers and model users and developers. Upper level management and the public may be interested in more general statements of model precision, and should be provided with such information along with model estimates. On the other hand, detailed studies addressing the significance and interactions among individual factors would likely be meaningful to model developers and some model users. They can use such data to interpret model results and to identify where to direct the efforts to improve models and factor values.

Analytical methods are faced with considerable difficulties in: obtaining the derivatives for many models; needing to assume mathematical (usually linear) relationships when obtaining estimates of derivatives by making small changes of factor values near their nominal or most likely values; and having large variances associated with most biophysical process models. Analytical methods are less demanding as computational resources, however the requirements mentioned above are never met by complex models simulating biophysical systems via process-based approaches. These have motivated the replacement of analytical methods by numerical and statistical approaches to SA.

Among the most used methods three classes can be identified: screening methods, regression-based methods, variance-based methods. The most often used screening method is the one proposed by Morris (1991), particularly effective in identifying the most important parameter in complex models with many parameters or with high computational requirements. Morris' method is based on the computation of a certain number of incremental ratios (elementary effects) for each factor and to averaging them to estimate the overall factor importance on model output(s) (Campolongo *et al.*, 2007). The second class includes the regression methods, which are based on the computation of standard or partial regression coefficients quantifying the effects of changing one parameter while keeping the others constant. Within this class, different methods can be used to generate the sample of factors combinations (needed to evaluate all parameters, even if one at the time) necessary to obtain the model evaluations and therefore to calculate the regression coefficients; here, Latin Hypercube Sampling (LHS), Random, and Quasi-Random LpTau is often used. The last class, the variance-based methods, includes the Fourier Amplitude Sensitivity Test (FAST) (Cukier *et al.*, 1978), its evolution the Extended FAST (E-FAST; Saltelli *et al.*, 1999), and the method of Sobol (Sobol, 1993). All methods belonging to this class computes total sensitivity indices for first and higher orders effects and are quite demanding in terms of computational time because of the high number of model evaluations needed for each model factor. FAST and E-FAST use transformation functions to sample the parameters space, assuming that factor probability distributions are uniform. As Sobol' does not use transformation functions it is more demanding computational resources and it needs *a priori* definition of parameter distributions.

Even if a method like Morris' could be implemented with reasonable ease in a proprietary system allowing a tight customization, the importance of accessing a variety of SA methods suggest to use of a reference library. The ease of access to SA resources in a specific modelling framework would allow to make SA an effective tool in model development and operational use.

In this paper we present a new generic software component for SA of biophysical models, implementing the most often used SA methods. The use of the Morris' method in two case studies in which spatially distributed SA was carried out for two different biophysical models is presented as sample application of the component.

2. MATERIALS AND METHODS

2.1. LUISA (Library Use Interface for Sensitivity Analysis)

LUISA (Library User Interface for Sensitivity Analysis) is a component developed with the goal of making the sensitivity analysis models implemented in the Simlab library (<http://simlab.jrc.ec.europa.eu/>) available via a user friendly application programming interface. The software is developed as a Microsoft .NET component making the Simlab library (which is usable in C, C++, Matlab and Fortran) available in the .NET platform.

LUISA allows the easy integration of sensitivity analysis capabilities into bio-physical model frameworks. Figure 1 shows the structure of the sensitivity analysis components. The SA interface component and the Simlab library can be used autonomously by third parties. The SA graphical user interface and the SA Model Runner extension are made available in the software development kit (SDK) as examples on how to extend/reuse the component.

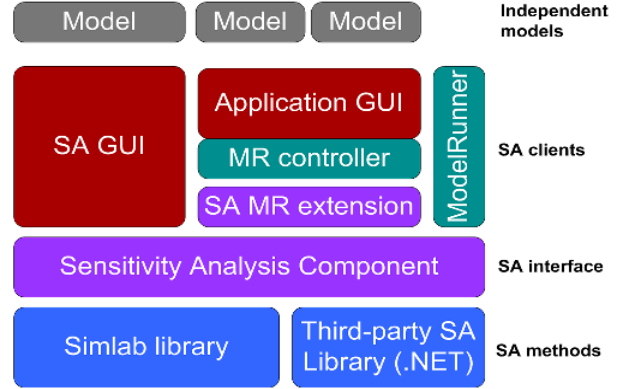


Figure 1. The sensitivity analysis components structure. MR is a software implementing a framework to link and run model components; its use is not mandatory. The use of the SA GUI is alternate to the use of the Model Runner via the Model-View-Controller design pattern in the sample projects provided.

Models to be analyzed are interfaced using the Adapter design pattern, hence by implementing a class (the adapter implementing the interface `IModelCaller`) made available in an autonomous component. The interface is made available in a different, discrete component because it is used by other components or applications. LUISA is available at <http://agsys.cra-cin.it/tools> together with the related SDK including help files and code documentation, and can be freely used and distributed by modellers and developers in their own applications. The license is reported in the documentation.

2.2. The Morris method for sensitivity analysis

The Morris method (Morris, 1991) is a one-factor-at-a-time sensitivity analysis method which is often used when the number of model parameters is large and the model simulations are quite time consuming. This method was used because of the need of performing spatially distributed sensitivity analysis, therefore needing to run a huge number of simulations. We always use this method as first SA analysis because of its convenience as above.

The Morris method calculates elementary effects due to each input factor using the following equation:

$$R_i(x_1, \dots, x_n, \Delta) = \frac{y(x_1, \dots, x_{i-1}, x_i + \Delta, x_{i+1}, \dots, x_n) - y(x_1, \dots, x_n)}{\Delta}$$

where $y(X)$ is the output, $X=(x_1, \dots, x_n)$ is the n -dimensional vector of factors being studied, Δ is a value between $1/(p-1)$ and $1-1/(p-1)$, p is the number of levels. The method samples values of X from the hyperspace Ω (identified by an n -dimensional p -level grid) and finally calculates mean (μ ; assessing the overall influence of the factor on $y(X)$) and standard deviation (σ ; estimating the totality of the higher order effects, i.e., non-linearity or interactions with other factors) (Saltelli et al., 2004) of all the R_i obtained for each factor. μ and σ are calculated over different trajectories, composed by individual one-factor-at-a-time experiments. The total number of model evaluations needed is $t(n+1)$, where t is the number of trajectories.

In this study, we used the revised version of the Morris method proposed by Campolongo et al. (2007). This evolution of the Morris method is based on a refined sampling strategy and provides μ^* instead of μ , by averaging the absolute values of the incremental ratios instead of the values themselves.

2.3. The case studies

Two illustrative case studies were carried out to present LUISA's functionalities and the potential of the implemented Morris' method. For the first case study, a spatially distributed SA for the rice growth model WARM (Confalonieri *et al.*, 2009a, b) applied throughout Europe was carried out. The model is based on a radiation use efficiency approach. The second case study was a SA for the generic crop simulator CropSyst (Stöckle *et al.*, 2003) for winter wheat in Italy. CropSyst is a cropping system simulation model; the sub-models used are the generic crop simulator. The crop simulator simulates growth as the minimum of the estimates made using a transpiration efficiency model and a radiation use efficiency model. The two models, implemented in the crop model library CropML (<http://agsys.cra-cin.it/tools/>), are linked to the MARS (Monitoring Agriculture with Remote Sensing) database (Micale and Genovese, 2004) of the European Commission - Joint Research Centre (Ispra, Italy). Spatial resolution of weather and management data was 50 km × 50 km, the standard of the Crop Growth Monitoring System (CGMS) of the European Commission (Micale and Genovese, 2004). For both models, the relevant output variable was aboveground biomass at physiological maturity (phenology parameters as estimated in a representative year, 2004). The cases are presented for illustrative purposes of the use of the library, hence the analysis is limited to two parameters only due to space constraints.

Parameters distributions (required by the Morris method) were retrieved as described in detail by Confalonieri *et al.* (2006) from the literature (van Diepen *et al.*, 1988; Kropff *et al.*, 1994; Donatelli *et al.*, 1997; Pannkuk *et al.*, 1998; Confalonieri and Bocchi, 2005; Boschetti *et al.*, 2006; Bechini *et al.*, 2006). A triangular distribution was used for all the parameters.

The Morris method was parameterized adopting seven as number of trajectories and four as number of levels.

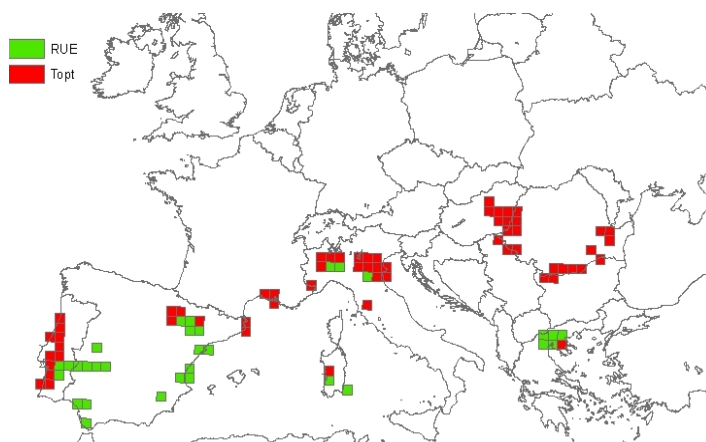


Figure 2. Main contributor map for the WARM rice model according to the Morris μ^* . RUE and Topt are maximum radiation use efficiency and optimum mean daily temperature for growth respectively.

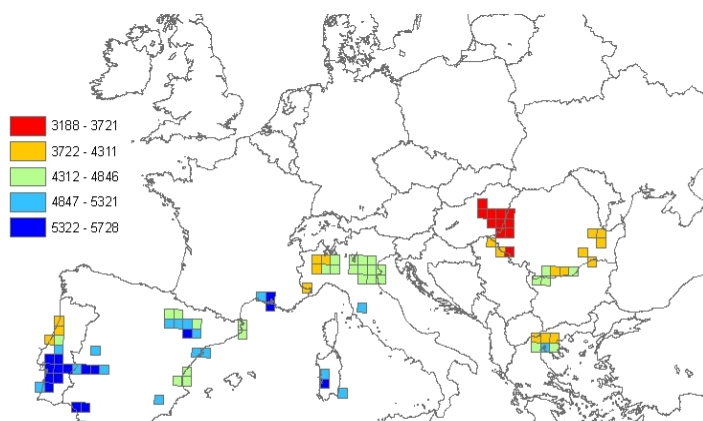


Figure 3. Value of the Morris μ^* for the WARM model parameter radiation use efficiency (RUE).

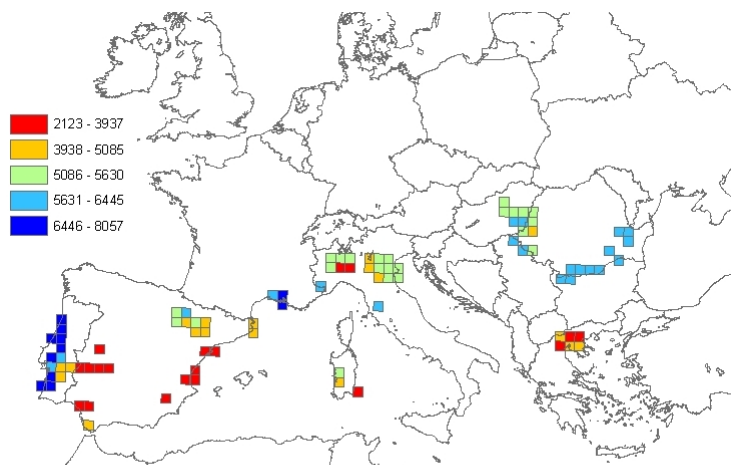


Figure 4. Value of the Morris μ^* for the WARM model parameter optimum mean daily temperature for growth (Topt).

3. RESULTS AND DISCUSSION

SA results are presented in two different types of map. The first type is the main-contributor map (Fig. 1,5), which display which is the most relevant model parameters for each cell of the 50 km × 50 km grid. The second type displays, for a certain model parameter, the values of the SA index Morris μ^* (Fig. 3,4,6,7).

3.1. Case study 1. Spatially distributed sensitivity analysis of the rice model WARM in Europe

Figure 2 shows the main contributor (most relevant model parameter) for each grid cell (only rice growing areas are coloured).

The WARM model is most sensitive to the parameter optimum mean daily temperature for growth (T_{opt}) where temperatures are lower than the optimum temperature for rice for a big part of the rice cycle. This is often related to areas characterized by high (for rice) latitudes (e.g., Eastern Europe countries, Northern Italy, France) or by maritime climate (e.g., Portugal).

On the contrary, maximum radiation use efficiency (RUE) is the parameter most relevant where both irradiative levels and temperatures are higher (e.g., Southern Spain, Sardinia, Greece). This can be explained considering the S-shaped function used for modelling the photosynthesis response to temperature (see CropML documentation): the thermal limitation factor assumes values which are in the region of the S-shaped function characterized by a plateau when average daily temperatures are high enough to get close to the value of T_{opt} . Under these conditions, RUE is more relevant also because high irradiative levels magnify the effect of variations in RUE values, the latter used to multiply radiation and therefore directly proportional to daily aboveground biomass accumulation.

Figures 3 and 4 present the values of the Morris μ^* for the WARM model parameters RUE and T_{opt} , respectively.

RUE relevance (Figure 3) follows a gradient which increases moving from North-East to South-West. North-Eastern grid cells are characterized by higher latitudes and continentality levels.

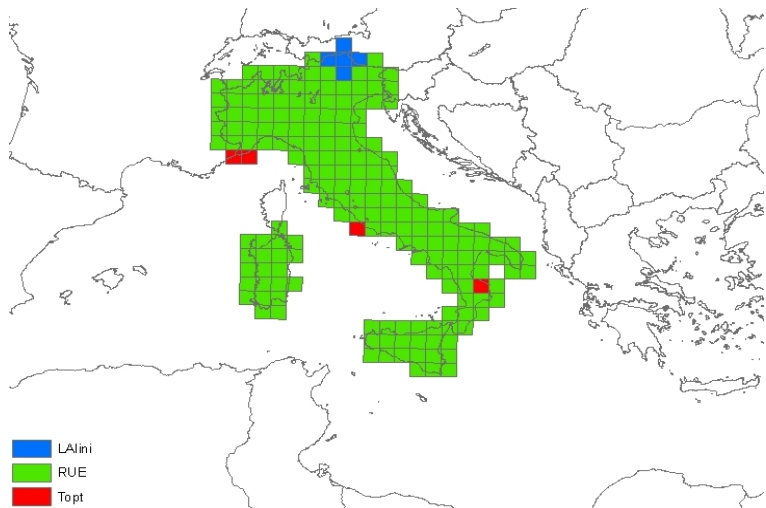


Figure 5. Main contributor map for the CropSyst model (winter wheat) according to the Morris μ^* . LAIni, RUE, and Topt are Initial leaf area index, maximum radiation use efficiency, and optimum mean daily temperature for growth, respectively.

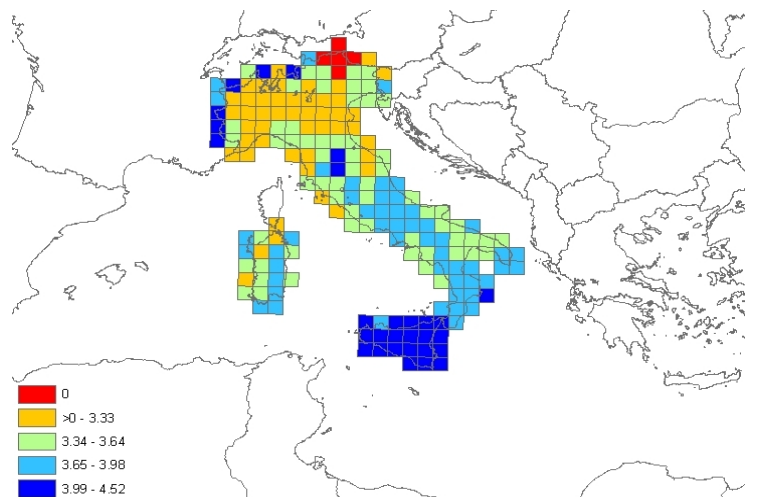


Figure 6. Value of the Morris μ^* for the CropSyst model parameter radiation use efficiency (RUE).

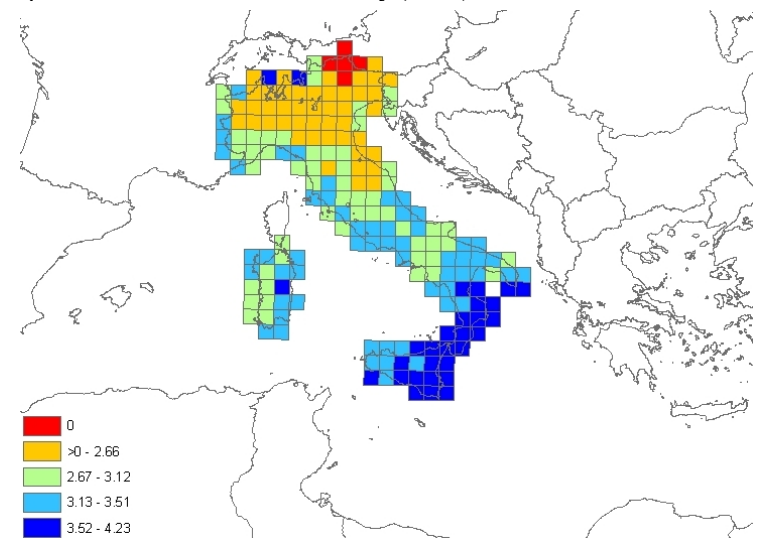


Figure 7. Value of the Morris μ^* for the CropSyst model parameter optimum mean daily temperature for growth (T_{opt}).

The parameter assumes more importance in influencing the model output where the irradiative levels are generally higher and more variable (higher values correspond to higher sensitivity due to the parameter).

Figure 4 shows the value of Morris μ^* for the parameter T_{opt} . The highest parameter's relevance is calculated for the grid cells where temperatures are lower (e.g., Portugal and North-Eastern rice producing Countries). Compared to RUE relevance (Figure 3), the distribution of Morris μ^* values is less homogeneous.

3.2. Case study 2. Spatially distributed sensitivity analysis of the generic crop simulator CropSyst for winter wheat in Italy

Figure 5 shows the main contributor (most relevant model parameter) for each grid cell. Compared to the map displaying the same results for the WARM model (Figure 2), the situation is more homogeneous. Radiation use efficiency (RUE) is almost always the parameter with the highest influence on aboveground biomass at physiological maturity. Optimum mean daily temperature for growth (T_{opt}) is the most relevant CropSyst parameter in few grid cells indicating variable temperature patterns (regions Liguria, Lazio and Calabria). Initial leaf area index (LAI_{ini}) is the most relevant in few North-Eastern areas, where the growing season is shorter and starts late in the season; a greater value of LAI_{ini} ensure a quicker start of the linear phase of growth.

RUE is most relevant in the Southern regions and in Sardinia (Figure 6), where irradiative levels are higher. The only exceptions are calculated especially for the North-Western grid cells, at the border with France, and two cells in Tuscany. These cells are in high elevation areas. The relevance of the parameter T_{opt} (Figure 7) follows a similar pattern to that described for RUE.

4. CONCLUSIONS

Analyzing biophysical models sensitivity to their parameters is crucial for an better understanding of their behaviour and applicability in specific conditions, thus supporting both their development and use. Rigorous analyses of model parameters relevance require the use of specific techniques, often based on sampling designs of parameters input space which are computational resource intensive. Sensitivity analysis should therefore be facilitated by dedicated support tools. This is related to the need of providing modern biophysical modelling environments with integrated tools for the execution of sensitivity analyses. An easy access to sensitivity analysis allows scientists to develop consistent models, avoiding problems related to over-parameterization. Also, it allows identifying the introduction of non-relevant modules in a specific modelling solution to be used in a specific context.

The LUISA component proved its suitability for running spatially distributed SA on two different biophysical models. The structure of the component allows an easy interfacing with biophysical model frameworks. Moreover, the user can select the more suitable SA method for a specific objective, considering the model complexity, the number of model parameters, and – more generally – the computational requests of the combination given by the system to simulate and the sensitivity analysis method.

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